Cumene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.04e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.17e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found
5-Ethylidene-2-norbornene
Measured: 7.40e-05
Predicted: 2.32e-04

Image not found
4-Vinylcyclohexene
Measured: 4.62e-04
Predicted: 3.42e-04

Image not found
Limonene
Measured: 7.77e-05
Predicted: 5.10e-05

Image not found
D-Limonene
Measured: 7.77e-05
Predicted: 5.10e-05

Image not found
gamma-Terpinene
Measured: 6.37e-05
Predicted: 4.78e-05

Image not found
Bis-(2-chloroethyl)sulfide
Measured: 4.32e-03
Predicted: 3.70e-03